

# Effect of surface anisotropy on the hysteretic properties of a magnetic particle

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We study the influence of surface anisotropy on the zero-temperature hysteretic properties of a small single-domain magnetic particle, and give an estimation of the anisotropy constant for which deviations from the Stoner-Wohlfarth model are observed. We consider a spherical particle with simple cubic crystalline structure, a uniaxial anisotropy for core spins and radial anisotropy on the surface, and compute the hysteresis loop by solving the local Landau-Lifshitz equations for classical spin vectors. We find that when the surface anisotropy constant is at least of the order of the exchange coupling, large deviations are observed with respect to the Stoner-Wohlfarth model in the hysteresis loop and thereby the limit-of-metastability curve, due to the non-uniform cluster-wise reversal of the magnetisation.

## I. STATEMENT OF THE PROBLEM

In this work, we deal with the effect of surface anisotropy on the hysteretic properties (hysteresis loop and limit-of-metastability curve, the so-called SW astroid [2]) of a single-domain spherical particle of simple cubic crystalline structure, uniaxial anisotropy in the core, and radial single-site anisotropy for spins on the boundary. We compute the hysteresis loop and thereby the critical field of this particle by solving, at zero temperature, the local Landau-Lifshitz equation (LLE) derived from the classical anisotropic Dirac-Heisenberg model in field (1). Doing this for different values of the polar angle  $\psi$  between the applied field and the core easy axis, renders the critical field as a function of  $\psi$ , that is the SW astroid. Finally, our model Hamiltonian reads [3]

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - (g\mu_B) \mathbf{H} \cdot \sum_{i=1}^{\mathcal{N}} \mathbf{S}_i - \sum_i K_i (\mathbf{S}_i \cdot \mathbf{e}_i)^2, \quad (1)$$

where  $\mathbf{S}_i$  is the unit spin vector on site  $i$ ,  $\mathbf{H}$  is the uniform magnetic field applied in a direction  $\psi$  with respect to the reference  $z$  axis,  $\mathcal{N}$  is the total number of spins;  $J > 0$  is the nearest-neighbour exchange coupling; the last term in (1) is the uniaxial anisotropy energy with easy axis  $\mathbf{e}_i$  and constant  $K_i > 0$ . Core spins have an easy axis along  $z$  and constant  $K_c$ , while surface spins have radial easy axes and constant  $K_s$ . In the sequel, we use the reduced parameters,  $j \equiv J/K_c$ ,  $k_s \equiv K_s/K_c$ .

The only free parameter of our model is the surface anisotropy constant  $k_s$ . So upon varying it we estimate its value at which deviations from the (macroscopic) Stoner-Wohlfarth model are observed. Details of the method used here and more results can be found in Ref. [3].

## II. RESULTS AND DISCUSSION

Fig. 1 shows that when  $k_s$  becomes comparable with  $j$ , the competition between exchange coupling and surface anisotropy produces large deviations from the SW model. Namely, the hysteresis loop exhibits multiple jumps, which can be attributed to the switching of different spherical shells of spins starting from surface down to the centre. The hysteresis loop is then characterised by two field values: One that marks the limit of metastability, called the *critical field* or the saturation field, and the other that marks the magnetization switching, and is called the *switching field* or the coercive field. In Fig. 2a we present the variation with the particle's diameter of the critical field [4] (in diamonds) obtained from the numerical solution of the LLE for  $j = 10^2$ , and (in circles) the SW critical field multiplied by the core-to-volume ratio, i.e.  $N_c/\mathcal{N}$ , analytically obtained upon assuming infinite exchange coupling. This figure also shows that for such a value of  $k_s$ , when the field is applied along the core easy axis, the critical field increases with the particle's size, and that for  $k_s = 1 = 10^{-2}j$  all hysteresis loops can be scaled with those rendered by the SW model.

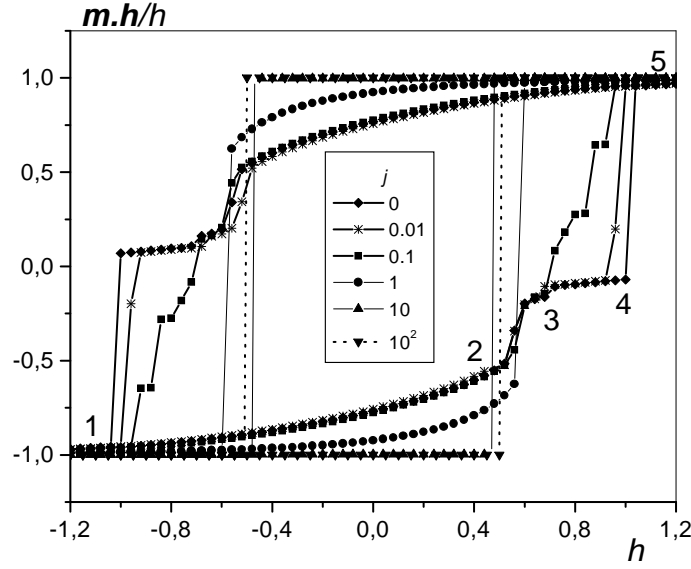


FIG. 1. Hysteresis loop for  $\psi = 0$ ,  $k_s = 1$  and different values of  $j$ .  $\mathcal{N} = 360$ .

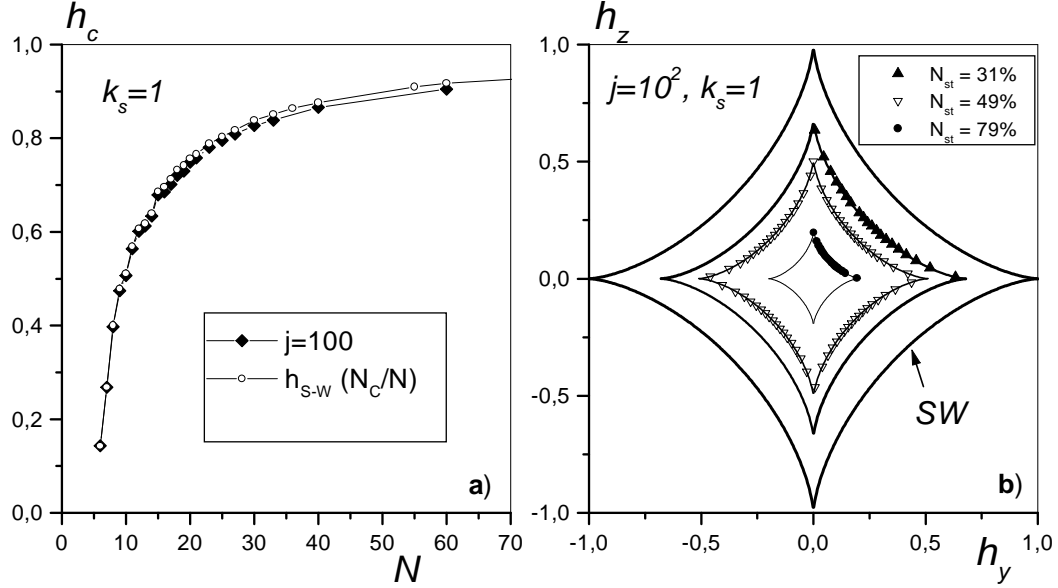


FIG. 2. a) (in diamonds) Switching field for  $k_s = 1$ ,  $j = 10^2$  versus the particle's diameter  $N$ . (in circles) SW switching field multiplied by  $N_c/\mathcal{N}$ . b) Astroid for  $k_s = 1$ ,  $j = 10^2$  for different values of the surface-to-volume ratio  $N_{st} \equiv N_s/\mathcal{N}$ .

On the other hand, these results clearly show that even in a large particle there still exist some magnetic inhomogeneities that lead to deviations from the SW hypothesis of uniform rotation, as this is only rigorously realized in an infinite system. Moreover, Fig. 2 shows that the critical field of a spherical particle with  $k_s = 1$  can be obtained from the SW model through a scaling with constant  $N_c/\mathcal{N}$ . One should also note that the astroid for all particle sizes falls inside that of SW, see Fig. 2b. Therefore, for  $k_s/j \sim 0.01$  our model renders hysteresis loops and limit-of-metastability curves that scale with the SW results for all values of the angle  $\psi$ , the scaling constant being  $N_c/\mathcal{N}$ , which is smaller than unity for a particle of any finite size. On the other hand, the critical field increases with the particle's size and tends to the SW critical field in infinite systems.

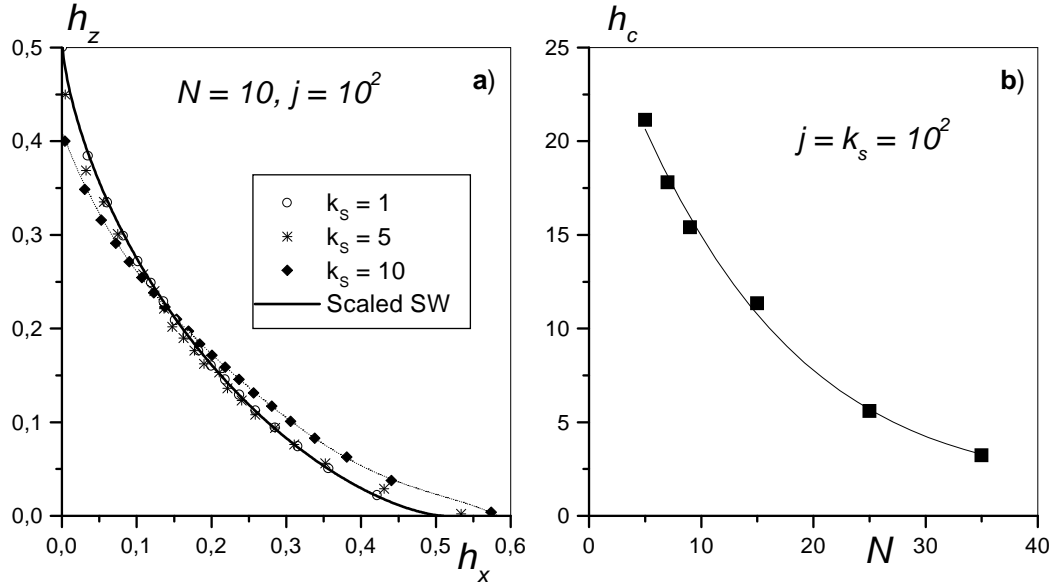


FIG. 3. a) Astroid for  $j = 10^2$ ,  $N = 360$  and different values of surface anisotropy constant  $k_s$ . The full dark line is the SW astroid scaled with  $N_c/N$ , but the dotted line is only a guide for the eye. b) Switching field versus the particle's diameter  $N$  for  $\psi = 0$ ,  $j = k_s = 10^2$ .

For larger values of  $k_s/j$ , but  $k_s/j \lesssim 0.2$ , we still have some kind of scaling but the corresponding constant now depends on  $\psi$ . This is reflected by a deformation of the limit-of-metastability curve. More precisely, as shown by Fig. 3a, the latter is depressed in the core easy direction and enhanced in the perpendicular direction. However, there is still only one jump in the hysteresis loop implying that the magnetization reversal can be considered as uniform. On the other hand, Fig. 3b shows that for  $k_s/j \sim 1$  there are two new features in comparison with the previous case (compare Fig. 2a): the values of the switching field are much higher, and more importantly, its behaviour as a function of the particle's size is opposite to that of the previous case, as now the field increases when the particle's size is decreased. For such high values of  $k_s$  ( $K_s \gg K_c$ ) surface spins are aligned along their easy axes, and because of the strong exchange coupling they also drive core spins in their switching process. Thus the smaller the particle the larger the surface contribution, and the larger the field required for a complete reversal of the particle's magnetization.

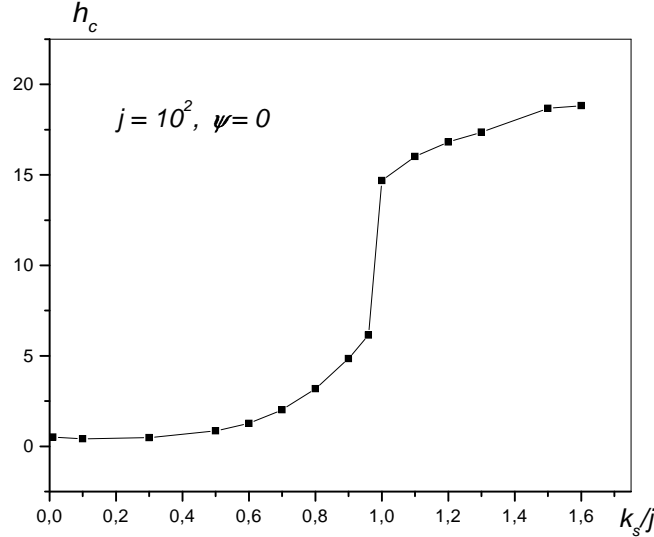


FIG. 4. Switching field versus the surface anisotropy constant for  $\psi = 0$ ,  $j = 10^2$ , and  $N = 10$ .

In Fig. 4  $h_c$  first slightly decreases for  $k_s/j \lesssim 0.1$  and then increases, and when  $k_s$  becomes of the order of  $j$  it jumps

to large values. This plot illustrates the different regimes discussed above according to the value of the ratio  $k_s/j$ . For an order of magnitude estimate of  $K_s$  and the critical field  $H_c$  at the point  $k_s/j = 1$ , consider a 4 nm spherical cobalt particle for which  $J \simeq 8$  meV,  $K_c \simeq 2.7 \times 10^6$  erg/cm<sup>3</sup>. Then,  $K_s \sim 10$  erg/cm<sup>2</sup>, and  $H_c \sim 5$  T, when the field is applied along the core easy axis.

### III. CONCLUSION

Considering the fact that experiments on nanoparticles show that the switching field does increase when the particle's size decreases (see e.g. [5] for cobalt particles), we may conclude that the anisotropy constant  $K_s$  is at least of the order of the exchange coupling  $J$ , inasmuch as we can assume radial anisotropy on the surface, as is usually done in the literature. Then, as discussed above, for such values of  $K_s$ , large deviations are observed with respect to the SW model in the hysteresis loop and thereby the limit-of-metastability curve, since in this case the magnetisation reverses its direction in a non-uniform manner via a progressive switching of spin clusters. So to deal with these features one has to resort to microscopic approaches such as the one used in this work. A work in progress applies the present technique to the cubo-octahedral cobalt particles with a diameter of about 3nm recently reported on in [6].

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  - [4] For  $k_s = 1$ , there is only one jump in the hysteresis loop and thus the critical field coincides with the switching field.
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